These are suggested (directed) answers to some of the basic questions that will need to be addressed during development of the Portland Harbor transport and fate (T&F) and food web models.

Model Purpose

1. Provide managers with information about possible long-term outcomes from various remediation options
2. Provide estimates of residue levels in species (e.g., sturgeon, great blue heron) for which empirical data are unlikely to be available.
3. Because so much empirical data will be available to support the ecological risk assessment, there may be little need for the model here

Model Elements

- A simple mass balance T&F model linked to food web models will be required. Such a linkage has been accomplished elsewhere.[1]
- The T&F model can be developed from several variations available in the literature, all of which have proven useful in situations similar to Portland Harbor.[2, 3]
- The food web models should be based on the form initially established by Gobas and subsequently improved by him and others.[4]
- To address the issue of receptor exposures while moving (foraging), divide the harbor into segments within the T&F model (see below), develop a similar food web model for each segment, and apportion exposure to a mobile receptor as a function of its estimated residence time in each segment.

Temporal Granularity & Scale

- The models must be dynamic (time-dependent) so that it is possible to track changes over time (in response to possible remedial alternatives) and to determine how long it will take the system to approach steady-state.[5]
- Steady-state only models are not acceptable.
- Both models will need to incorporate seasonally varying data (e.g., river flow rate, water temperature, etc.). A monthly period will provide a reasonable balance between model resolution and the amount of data generated.
- The time increment (*dt*) must be sufficiently small to capture changes which occur within the course of a time unit (i.e., a month).
- Because of the half-life of some of the contaminants involved, the model should be capable of estimating forward 20-25 years, on a monthly basis.

Spatial Granularity & Scale

- A multi-segment model is required.[6, 7]
- The model domain should extend from river mile (RM) 11 to RM 2, with a separate compartment for Swan Island Lagoon.

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1 Mackay D, Sang S, Vlahos P, Diamond M, Gobas F and Dolan D. 1994. A rate constant model of chemical dynamics in a lake ecosystem: PCBs in Lake Ontario. *Journal of Great Lakes Research* 20(4): 625-642.
2 Davis JA. 2003. The long term fate of PCBs in San Francisco Bay. RMP Technical Report: SFEI Contribution 47. San Francisco Estuary Institute, Oakland, CA.
3 Davis JA. 2004. The long term fate of PCBs in San Francisco Bay. *Environmental Toxicology and Chemistry* 23(10): 2396-2409.
4 Arnot JA and Gobas FAPC. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. *Environmental Toxicology and Chemistry* 23(10): 2343-2355.
5 Mackay D. 2001. Multimedia Environmental Models: The Fugacity Approach, Second Edition. 2001. Lewis Publishers, Boca Raton, FL. p.212.
6 See Mackay (2001), p. 210.
7 Mackay D and Hickie B. 2000. Mass balance model of source apportionment, transport and fate of PAHs in Lac Saint Louis, Quebec. *Chemosphere* 41: 681-692.

- This domain should be divided into ½-mile segments, at right-angles to the river flow (i.e., bank-to-bank).
- Other segmentation patterns (parallel to flow, by habitat, etc.) may be considered after the basic T&F model is built.

Flow Regimes

- USGS data are available from RM 12.8 to provide measures of flow on a monthly basis for 30+ years.
- During the summer low flow period, flow reversals and intrusion of Columbia River water can occur. The T&F model should be able to accommodate these phenomena at least to the point where there impact on contaminant movement can be assessed.

Loadings

- The T&F model should make provision loads that enter Segment 1 from upstream sources (those above RM 11).
- The T&F model should also make provision for including loadings from various sources (e.g., overland, outfalls, groundwater, etc.), even if the quantities of loadings from such sources are currently unknown.

Contaminants

- Polychlorinated biphenyls. As there are numerous congeners, it may be expedient to use PCB 118 as a surrogate for this group.[8]
- Polycyclic aromatic hydrocarbons. Again, another large group - a subset will need to be identified for modeling, as was done for San Francisco Bay.[9, 10] It appears that the metabolism of these contaminants by some aquatic species can be addressed within the type of food web model contemplated here.[11]
- Pesticides, represented by DDE, since it is the more toxic, persistent, and bioaccumulative of by-product of DDT. Using ΣDDT is not recommended as this can obscure important physicochemical differences among DDT, DDE, and DDD.
- These models are not designed to address metals mechanistically. Metals that are actually expected to biomagnify may be only secondary cocern.[12] Modelling methylmercury would require a different, specialized, model, which may not be justified at this time.

Food Web Complexity

- The Arnot and Gobas formulation of the Gobas food web model is preferred.[13, 14]
- An overly detailed food web, with numerous species, is likely to exceed both the availability of site-specific data (i.e., data from 6 fish aren't enough), as well as literature-derived physiological data.
- As the models' primary purpose is to inform remediation decisions and not precisely predict tissue residues, a simplified food web, encompassing representative pelagic and benthic species, should be sufficient at this time.

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8 See Davis (2003, 2004).

9 Greenfield BK and Davis JA. 2004. A simple mass balance model for PAH fate in the San Francisco Estuary. RMP Technical Report, SFEI Contribution 115. San Francisco Estuary Institute, Oakland, CA.

10 Greenfield BK and Davis JA. 2005. A PAH fate model for San Francisco Bay. *Chemosphere* 60: 515-530.

11 Stevenson RW. 2003. Development and application of a model describing the bioaccumulation and metabolism of polycyclic aromatic hydrocarbons in a marine benthic food web. M.S. thesis, School of Resource and Environmental Management, Simon Fraser University, British Columbia, Canada.

12 Reinfelder JR, Fisher NS, Luoma SN, Nichols JW and Wang WX. 1998. Trace element trophic transfer in aquatic organisms: a critique of the kinetic model approach. Science of the Total Environment 219(2-3): 117-135.

13 See #4.

14 Gobas F and Wilcockson J. 2003. San Francisco Bay PCB food-web model. RMP Technical Report, SFEI Contribution 90. San Francisco Estuary Institute, Oakland, CA.

- A food web model in each segment can address the issue of receptor range and movement.
- Using matrix methods, it is possible to include scavenging and/or cannibalism feeding behaviors in these food webs.[15] However, to minimize model complexity, these feeding relationships should be excluded unless there is a compelling reason to do otherwise.
- Fluctuations in dietary preference can be addressed by normalizing dietary fractions across a "menu" of possible food items.[16]

Data Availability

- The initial goal is a set of integrated working models that capture the principle features of abiotic and biotic T&F within the harbor. Achieving working models should not be held hostage to data availability.
- The models should therefore be initially built-out with available site-specific data and appropriate data from the literature. Data gaps should be both identified and filled with information based on best professional judgment. Placeholders should be left for key items (e.g., loadings) which are already known to be important but may not be quantified for some time.
- Sensitivity analysis should be used to narrow our interest in data gaps to those which have the greatest impact on model performance.
- These data gaps can then be addressed in greater detail as the models progress through various editions and refinements.

Model Platform

- The key determinant of which platform (i.e., software) to use is transparency, which is defined as the ability for an informed user to follow (if desired) every step of model operation. "Balck box" approaches are to be minimized, if not simply avoided.
- The models should be written in VBA™, with input/output through Excel™ spreadsheets, with "elegant" or otherwise "streamlined" coding is discouraged in favor of transparency.
- The one area where some transparency may be sacrificed is with respect to analysis of uncertainty and sensitivity. For these, use of a Monte Carlo software (e.g., CrystalBall®, @Risk®, etc.) capable of linking to both Excel™ spreadsheets and VBA™ should be considered. This would considerably simplify the currently cumbersome approach to both of these analyses.

15 Sharpe S and Mackay D. A framework for evaluating bioaccumulation in food webs. *Environmental Science & Technology* 34(12): 2373-2379.

16 USEPA. 2003. Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) Modeling System. Volume I: Modeling System and Science. EPA 530-D-03-001a. Office of Research and Development / Office of Solid Waste, U.S. Environmental Protection Agency, Washington, DC. Section 12, page 12-8.